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Trotter–Kato product formula and fractional powers of self-adjoint generators

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Abstract

Let A and B be non-negative self-adjoint operators in a Hilbert space such that their densely defined form sum $H = A \dot{+} B$ obeys $\mathrm{dom}(H^\alpha) \subseteq \mathrm{dom}(A^\alpha) \cap \mathrm{dom}(B^\alpha)$ for some $\alpha \in (1/2, 1)$. It is proved that if, in addition, A and B satisfy $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$, then the symmetric and non-symmetric Trotter–Kato product formula converges in the operator norm:

$$||(e^{-tB/2n}e^{-tA/n}e^{-tB/2n})^n - e^{-tH}|| = O(n^{-(2\alpha-1)})$$

$$||(e^{-tA/n}e^{-tB/n})^n - e^{-tH}|| = O(n^{-(2\alpha-1)})$$

uniformly in $t \in [0, T]$, $0 < T < \infty$, as $n \to \infty$, both with the same optimal error bound. The same is valid if one replaces the exponential function in the product by functions of the Kato class, that is, by real-valued Borel measurable functions $f(\cdot)$ defined on the non-negative real axis obeying $0 \leqslant f(x) \leqslant 1$, $f(0) = 1$ and $f'(+0) = -1$, with some additional smoothness property at zero. The present result improves previous ones relaxing the smallness of B^α with

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respect to A^α to the milder assumption $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ and extending essentially the admissible class of Kato functions.

Keywords: Trotter–Kato product formula; Operator norm convergence; Fractional powers

1. Introduction

In the present paper we deal with the operator-norm convergence of the Trotter–Kato product formula, which may have applications in quantum and in statistical mechanics.

Let A and B be two non-negative self-adjoint operators in a Hilbert space $\mathfrak{H}$ such that $\mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2})$ is dense in $\mathfrak{H}$. By H we denote the form-sum of A and B, i.e.

$$H = A \dot{+} B$$

which is a non-negative self-adjoint operator in the Hilbert space $\mathfrak{H}$. Obviously, one has $\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2})$. Further, we consider the Kato functions: they are real-valued Borel measurable functions f on $[0, \infty)$ satisfying

$$0 \leqslant f(x) \leqslant 1, \quad x \in [0, \infty), \quad f(0) = 1, \quad f'(+0) = -1,$$

$$0 \leqslant g(x) \leqslant 1, \quad x \in [0, \infty), \quad g(0) = 1, \quad g'(+0) = -1.$$

Typical examples of the Kato functions are

$$f(x) = e^{-x} \quad \text{and} \quad f(x) = (1 + k^{-1}x)^{-k}, \quad k > 0. \tag{1.1}$$

In two remarkable papers [6,7], Kato has shown that these assumptions are enough to prove

$$s - \lim_{n \to \infty} (f(tA/n)g(tB/n))^n = e^{-tH}$$

uniformly in $t \in [0, T]$, $0 < T < \infty$. In the following we call a relation of this type a Trotter–Kato product formula. Naturally the question arises whether under suitable conditions the strong convergence of the Trotter–Kato product formula can be improved to the operator-norm convergence with a convergence rate estimate. Indeed this is possible. Beginning with Rogava [16] the operator-norm convergence with different convergence rates was verified in [8–14]. However, all these convergence rates are not optimal except the cases studied in [12,14]. In [11,12] some of ideas of Chernoff [2,3], have been used to prove that in the case $\mathrm{dom}(H) \subseteq \mathrm{dom}(A) \cap \mathrm{dom}(B)$, which means that the algebraic sum $H = A + B$ is self-adjoint, the optimal error bound is $O(n^{-1})$. In [14] the conditions are formulated on the fractional powers A^α, B^α, for $\alpha \in (1/2, 1]$. They lead to the optimal convergence rate $O(n^{-2(\alpha-1)})$.

The aim of the present paper is to study, in a sense, an intermediate case. We assume

$$\mathrm{dom}(H^\alpha) \subseteq \mathrm{dom}(A^\alpha) \cap \mathrm{dom}(B^\alpha) \tag{1.2}$$

for some $\alpha \in (1/2, 1)$. This assumption is stronger than the natural condition $\mathrm{dom}(H^{1/2}) \subseteq \mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2})$, which is always satisfied, but weaker than the assumption $\mathrm{dom}(H) \subseteq \mathrm{dom}(A) \cap \mathrm{dom}(B)$ used in [11] and [12]. Notice that comparing to [14] we do not demand the smallness of B^α with respect to A^α. We assume that the Kato functions further fulfill the conditions

$$|f|_{2\alpha} := \sup_{x>0} \frac{|f(x) - 1 + x|}{x^{2\alpha}} < +\infty, \quad \alpha \in (0, 1], \tag{1.3}$$

$$|g|_{2\alpha} := \sup_{x>0} \frac{|g(x) - 1 + x|}{x^{2\alpha}} < +\infty, \quad \alpha \in (0, 1]. \tag{1.4}$$

It is easily seen that (1.3) and (1.4) are in fact conditions at the neighborhood of zero. We set

$$m_f(x) := \sup_{y \in [x, \infty)} f(y), \quad x > 0.$$

Notice that examples (1.1) satisfy condition (1.3) and $m_f(x) < 1$ for $x > 0$. The aim of this note is to prove the following statement:

Theorem 1.1. *Let A and B be non-negative self-adjoint operators and let $H := A \dot{+} B$ be their form sum. Assume that for some $\alpha \in (1/2, 1)$ condition* (1.2) *is satisfied. Further, let f and g be Kato functions which obey conditions* (1.3) *and* (1.4)*. If in addition one has $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ and $m_f(x) < 1$ for $x > 0$, then for any finite interval $[0, T]$ there is a constant $C_{T,2\alpha-1} > 0$ such that*

$$\|(f(tA/2n)g(tB/n)f(tA/2n))^n - e^{-tH}\| \leqslant C_{T,2\alpha-1} \frac{1}{n^{2\alpha-1}} \tag{1.5}$$

for $t \in [0, T]$ and $n = 1, 2, \ldots$.

Estimate (1.5) gives the ultimate error bound for the convergence rate, which can be seen from an example given in [17]. Formula (1.5) remains true with the same error bound, when $f(\tau A/2)g(\tau B)f(\tau A/2)$, where $\tau = t/n$, is replaced by related families of the form $f(\tau A)^{1/2} g(\tau B) f(\tau A)^{1/2}$, $g(\tau B)^{1/2} f(\tau A)\, g(\tau B)^{1/2}$, $g(\tau B) f(\tau A)$, $f(\tau A)\, g(\tau B)$, $g(\tau B/2) f(\tau A)\, g(\tau B/2)$ where $\tau \geqslant 0$. We note further that Theorem 1.1 improves the previous result in [14] where the same optimal convergence rate $O(n^{-(2\alpha-1)})$ was obtained but under stronger conditions on the operators A and B and on the Kato functions f and g, for details see Section 7. Notice also that Theorem 1.1 treats a case which is not covered by [11,12]. Nevertheless, setting formally $\alpha = 1$ in Theorem 1.1 the assumptions and results of that theorem turn into those ones of [11,12], except for the assumption $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ which is superfluous there. In [8] it is conjectured that this condition can be dropped for $\alpha \in (1/2, 1]$. However, the proof of this conjecture remains still open. By the way condition $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ implies $\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2})$ which guarantees the density of $\mathrm{dom}(H^{1/2})$ in $\mathfrak{H}$.

The proof of Theorem 1.1 relies again on ideas of Chernoff [2,3] and follows in many aspects [11,12]. Theorem 2.1 in Section 2 can be regarded as an operator-norm variant of Chernoff's approach, which, in contrast to [15], gives error-bound estimates. In particular, it generalizes a result of [11]. In Section 3 we prove some estimates which are necessary in the following using results from [11]. The main theorem announced in the introduction is proved in Section 4. In Section 6, an example is given which illustrates the situation of our main theorem. Finally, in Section 7 we make some remarks on the obtained result.

2. Convergence theorem

We start with a lemma, which is proven using the standard Dunford–Taylor operator calculus.

Lemma 1. *Let K and L be non-negative self-adjoint operators on the Hilbert space $\mathfrak{H}$. Then*

$$||e^{-K} - e^{-L}|| \leqslant N||(I+K)^{-1} - (I+L)^{-1}||$$

with a constant $N > 0$ independent of operators K and L.

Proof. By the Dunford–Taylor representation for exponentials we find

$$e^{-K} - e^{-L} = \frac{1}{2\pi i}\int_\Gamma dz e^{-z}((z-K)^{-1} - (z-L)^{-1}), \tag{2.1}$$

where the contour Γ is given by $\Gamma = \Gamma_0 \cup \Gamma_\infty$ with

$$\Gamma_0 = \{z \in \mathbb{C} : z = e^{i\varphi},\ \pi/4 \leqslant \varphi \leqslant 2\pi - \pi/4\},$$

$$\Gamma_\infty = \{z \in \mathbb{C} : z = re^{\pm i\pi/4},\ r \geqslant 1\}.$$

From (2.1) we find the representation

$$e^{-K} - e^{-L} = \frac{1}{2\pi i}\int_\Gamma dz e^{-z}(I+K)(z-K)^{-1} \times ((I+L)^{-1} - (I+K)^{-1})(I+L)(z-L)^{-1}. \tag{2.2}$$

Since

$$(I+K)(z-K)^{-1} = -I + (1+z)(z-K)^{-1}$$

one gets the estimate

$$||(I+K)(z-K)^{-1}|| \leqslant 1 + \frac{1+|z|}{\mathrm{dist}(z,\mathbb{R}_+)}.$$

Setting

$$N_\Gamma := \sup_{z\in\Gamma} \frac{1+|z|}{\mathrm{dist}(z,\mathbb{R}_+)} < \infty$$

we find

$$\sup_{z\in\Gamma} ||(I+K)(z-K)^{-1}|| \leqslant (1+N_\Gamma), \tag{2.3}$$

where the constant N_Γ depends only on Γ but not on the operator K. Similarly, from (2.3) one also gets

$$\sup_{z\in\Gamma} ||(I+L)(z-L)^{-1}|| \leqslant (1+N_\Gamma).$$

Using these estimates, we find from (2.2) that

$$||e^{-K} - e^{-L}|| \leqslant N||(I+K)^{-1} - (I+L)^{-1}||$$

with a constant

$$N := \frac{1}{2\pi}(1+N_\Gamma)^2 \int_\Gamma |dz|\,|e^{-z}|$$

depending only on the contour Γ. □

To prove the main theorem we shall use, as in [11,12], an operator norm version of Chernoff's theorem with error bound, which partly improves Lemma 2.1 of [11] in the case $\varrho < 1$.

Theorem 2.1. *Let $\{F(\tau)\}_{\tau\geqslant 0}$ be a family of non-negative self-adjoint contractions on $\mathfrak{H}$ such that $F(0) = I$ and let*

$$S(\tau) := \frac{I - F(\tau)}{\tau}, \quad \tau > 0.$$

Assume $\varrho \in (0,1)$. *Then there is a constant* $M_\varrho > 0$ *such that the estimate*

$$\|(I + tS(\tau))^{-1} - (I + tH)^{-1}\| \leqslant M_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.4}$$

holds for $\tau, t \in (0,1]$ *with* $0 < \tau \leqslant t$, *if and only if there is a constant* $C_\varrho > 0$ *such that the estimate*

$$\|F(\tau)^{t/\tau} - e^{-tH}\| \leqslant C_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.5}$$

is valid for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$.

Proof. Assume (2.4). By Lemma 1 there is a constant $N > 0$ such that

$$\|e^{-tS(\tau)} - e^{-tH}\| \leqslant N \|(I + tS(\tau))^{-1} - (I + tH)^{-1}\|$$

for $\tau, t > 0$. Using (2.4) we obtain

$$\|e^{-tS(\tau)} - e^{-tH}\| \leqslant N M_\varrho \left(\frac{\tau}{t}\right)^\varrho$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant 1$. Since

$$\sup_{x \in [0,1]} |x^r - e^{-r(1-x)}| \leqslant \frac{1}{r}, \quad r \geqslant 1,$$

we find

$$\|F(\tau)^{t/\tau} - e^{-tS(\tau)}\| \leqslant \frac{\tau}{t}$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. By the inequality

$$\|F(\tau)^{t/\tau} - e^{-tH}\| \leqslant \|F(\tau)^{t/\tau} - e^{-tS(\tau)}\| + \|e^{-tS(\tau)} - e^{-tH}\|$$

we finally get

$$\|F(\tau)^{t/\tau} - e^{-tH}\| \leqslant \frac{\tau}{t} + N M_\varrho \left(\frac{\tau}{t}\right)^\varrho$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. Since $\frac{\tau}{t} \leqslant (\frac{\tau}{t})^\varrho$ for $0 < \tau \leqslant t$, $\varrho \in [0,1]$, we obtain

$$\|F(\tau)^{t/\tau} - e^{-tH}\| \leqslant (1 + N M_\varrho) \left(\frac{\tau}{t}\right)^\varrho$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. Setting $C_\varrho := 1 + N M_\varrho$ we have verified (2.5).

To prove the converse we use the representation

$$(I + tS(\tau))^{-1} - (I + tH)^{-1} = \int_0^\infty dx\, e^{-x}(e^{-xtS(\tau)} - e^{-xtH})$$

for $\tau, t > 0$. We have

$$(I + tS(\tau))^{-1} - (I + tH)^{-1} = \sum_{n=0}^{\infty} \int_n^{n+1} dx\, e^{-x}(e^{-xtS(\tau)} - e^{-xtH})$$

for $\tau, t > 0$. By the substitution $x = y + n$ we obtain

$$\begin{aligned}(I + tS(\tau))^{-1} &- (I + tH)^{-1} \\ &= \sum_{n=0}^{\infty} e^{-n} \int_0^1 dy\, e^{-y}(e^{-(y+n)tS(\tau)} - e^{-(y+n)tH})\end{aligned}$$

for $\tau, t > 0$. Since

$$\begin{aligned}e^{-(y+n)tS(\tau)} &- e^{-(y+n)tH} \\ &= (e^{-ntS(\tau)} - e^{-ntH})e^{-ytS(\tau)} + e^{-ntH}(e^{-ytS(\tau)} - e^{-ytH})\end{aligned}$$

and

$$e^{-ntS(\tau)} - e^{-ntH} = \sum_{k=0}^{n-1} e^{-ktS(\tau)}(e^{-tS(\tau)} - e^{-tH})e^{-(n-k-1)tH}$$

we get

$$\begin{aligned}(I + tS(\tau))^{-1} &- (I + tH)^{-1} \\ &= \sum_{n=0}^{\infty} e^{-n}\Bigg\{\sum_{k=0}^{n-1} e^{-ktS(\tau)}(e^{-tS(\tau)} - e^{-tH})e^{-(n-k-1)tH} \int_0^1 dy\, e^{-y}\, e^{-ytS(\tau)} \\ &\quad + \int_0^1 dy\, e^{-y}\, e^{-ntH}(e^{-ytS(\tau)} - e^{-ytH})\Bigg\}.\end{aligned}$$

Hence we obtain the estimate

$$\begin{aligned}&||(I + tS(\tau))^{-1} - (I + tH)^{-1}|| \\ &\quad \leqslant \sum_{n=0}^{\infty} e^{-n}\left\{n||e^{-tS(\tau)} - e^{-tH}|| + \int_0^1 dy\, e^{-y}\, ||e^{-ytS(\tau)} - e^{-ytH}||\right\}\end{aligned} \tag{2.6}$$

for $\tau, t > 0$. By assumption (2.5) we have the estimate

$$||e^{-tS(\tau)} - e^{-tH}|| \leqslant C_\varrho \left(\frac{\tau}{t}\right)^\varrho \tag{2.7}$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. Further, we use the decomposition

$$\int_0^1 dy\, e^{-y}\, ||e^{-ytS(\tau)} - e^{-ytH}|| = \int_{\tau/t}^1 dy\, e^{-y}\, ||e^{-ytS(\tau)} - e^{-ytH}|| + \int_0^{\tau/t} dy\, e^{-y}\, ||e^{-ytS(\tau)} - e^{-ytH}||. \tag{2.8}$$

Setting $t' = yt$ one has $\tau \leqslant t'$ if $\tau/t \leqslant y$. Hence by assumption (2.5) we obtain

$$||e^{-ytS(\tau)} - e^{-ytH}|| \leqslant C_\varrho \left(\frac{\tau}{ty}\right)^\varrho$$

for $\tau, t, y \in (0,1]$ and $\tau/t \leqslant y$. This yields the estimate

$$\int_{\tau/t}^1 dy\, e^{-y}\, ||e^{-ytS(\tau)} - e^{-ytH}|| \leqslant C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} \left(\frac{\tau}{t}\right)^\varrho \tag{2.9}$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. For $\varrho < 1$ one obviously has

$$\int_0^{\tau/t} dy\, e^{-y}\, ||e^{-ytS(\tau)} - e^{-ytH}|| \leqslant 2\left(\frac{\tau}{t}\right)^\varrho \tag{2.10}$$

for $\tau, t \in [0,1]$ with $0 < \tau \leqslant t$. Taking into account (2.9) and (2.10) we obtain from (2.8) the estimate

$$\int_0^1 dy\, e^{-y}\, ||e^{-ytS(\tau)} - e^{-ytH}|| \leqslant \left(C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} + 2\right)\left(\frac{\tau}{t}\right)^\varrho \tag{2.11}$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. Finally, using (2.7) and (2.11) we get from (2.6) the estimate

$$||(I + tS(\tau))^{-1} - (I + tH)^{-1}|| \leqslant \sum_{n=0}^\infty e^{-n} \left\{ nC_\varrho + C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} + 2 \right\} \left(\frac{\tau}{t}\right)^\varrho$$

for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. Setting

$$M_\varrho := \sum_{n=0}^\infty e^{-n} \left\{ n\, C_\varrho + C_\varrho \int_0^1 dy\, e^{-y} y^{-\varrho} + 2 \right\}$$

we have verified (2.4). $\square$

We note that in [11] it was shown that for $\varrho = 1$ condition (2.4) implies (2.5). It is unclear whether in this case the converse is also true. Note also that setting $\tau = t/n$, $n = 1, 2, \ldots$, estimate (2.5) transforms into

$$||F(t/n)^n - e^{-tH}|| \leqslant C_\varrho \frac{1}{n^\varrho}$$

for $t \in (0, 1]$ and $n = 1, 2, \ldots$. However, this is nothing else but an operator norm estimate for a chosen family of contractions $F(\tau)$.

3. Auxiliary estimates

We are going to apply Theorem 2.1 to the family

$$F(\tau) := f(\tau A/2)g(\tau B)f(\tau A/2), \quad \tau > 0.$$

In the following we use notations which essentially go back to [11,12] but which are slightly modified. We set

$$\begin{aligned} A_\tau &:= \frac{I - f(\tau A)}{\tau}, \quad \tau > 0, \\ B_\tau &:= \frac{I - g(\tau B)}{\tau}, \quad \tau > 0, \\ K_\tau &:= B_\tau + A_{\tau/2} - \frac{\tau}{4} A_{\tau/2}^2, \quad \tau > 0. \end{aligned}$$

One has $K_\tau \geqslant 0$ and

$$S(\tau) = K_\tau + \frac{\tau^2}{4} A_{\tau/2} B_\tau A_{\tau/2} - \frac{\tau}{2}(B_\tau A_{\tau/2} + A_{\tau/2} B_\tau)$$

for $\tau > 0$. We set

$$\begin{aligned} Q_\tau := &\frac{\tau^2}{4}(I + K_\tau)^{-1/2} A_{\tau/2} B_\tau A_{\tau/2} (I + K_\tau)^{-1/2} \\ &- \frac{\tau}{2}(I + K_\tau)^{-1/2}(B_\tau A_{\tau/2} + A_{\tau/2} B_\tau)(I + K_\tau)^{-1/2}, \quad \tau > 0, \end{aligned}$$

so that

$$I + S(\tau) = (I + K_\tau)^{1/2}(I + Q_\tau)(I + K_\tau)^{1/2}, \quad \tau > 0.$$

Our next aim is to prove several estimates which we need for the proof of the main theorem.

Lemma 2. *Let A and B be non-negative self-adjoint operators. If f and g are Kato functions, then one has*

$$||B_\tau^{1/2}(I + K_\tau)^{-1/2}|| \leqslant ||(I + B_\tau)^{1/2}(I + K_\tau)^{-1/2}|| \leqslant 1$$

and

$$||A_{\tau/2}^{1/2}(I+K_\tau)^{-1/2}|| \leqslant \sqrt{2}\left|\left|\left(I+\frac{1}{2}A_{\tau/2}\right)^{1/2}(I+K_\tau)^{-1/2}\right|\right| \leqslant \sqrt{2}$$

for $\tau > 0$. *Moreover, the operator* $I + Q_\tau$ *has a bounded inverse for each* $\tau > 0$ *and the norm of its inverse operator is uniformly estimated by*

$$||(I+Q_\tau)^{-1}|| \leqslant \frac{1}{2}(3+\sqrt{5})$$

for $\tau > 0$.

Proof. The proof can be obtained from [11] by making the replacements $A \leftrightarrow B$ and $f \leftrightarrow g$. $\square$

Lemma 3. *Let* A *and* B *be non-negative self-adjoint operators. If* f *and* g *are Kato functions and* $m_f(x) < 1$ *for* $x > 0$, *then there are constants* $C_A > 0$ *and* $C_0 > 0$ *such that*

$$||(I+S(\tau))^{-1/2}u|| \leqslant C_A\,||(I+A)^{-1/2}u|| + C_0\,||u||\,\tau^{1/2} \tag{3.1}$$

for $u \in \mathfrak{H}$ *and* $\tau > 0$.

Proof. Using Lemma 2 we get

$$||(I+S(\tau))^{-1/2}u|| \leqslant \sqrt{\frac{3+\sqrt{5}}{2}}||(I+K_\tau)^{-1/2}u||$$

for $u \in \mathfrak{H}$ and $\tau > 0$. Since $K_\tau \geqslant \frac{1}{2}A_{\tau/2}$ we find

$$||(I+S(\tau))^{-1/2}u|| \leqslant \sqrt{3+\sqrt{5}}||(I+A_{\tau/2})^{-1/2}u||$$

for $u \in \mathfrak{H}$ and $\tau > 0$. Obviously, there is a constant $\delta > 0$ such that $|(1-f(x))x^{-1} - 1| > 1/2$ for $x \in (0,\delta)$. Hence

$$1 - f(x) \geqslant \frac{1}{2}x$$

for $x \in (0,\delta)$, which yields

$$1 - f(x) \geqslant \frac{1}{2}x\,\chi_{(0,\delta)}(x) + (1 - m_f(\delta))\chi_{[\delta,\infty)}(x)$$

for $x>0$, where $\chi_{(0,\delta)}(\cdot)$ and $\chi_{[\delta,\infty)}(\cdot)$ are the characteristic functions of the intervals $(0,\delta)$ and $[\delta,\infty)$, respectively. Hence we find

$$A_{\tau/2} \geqslant \frac{1}{2} A E_A([0, 2\delta/\tau)) + 2\frac{1-m_f(\delta)}{\tau} E_A([2\delta/\tau, \infty))$$

for $\tau>0$, where $E_A(\cdot)$ is the spectral measure of A. Therefore we obtain

$$\begin{aligned} &||(I+S(\tau))^{-1/2}u|| \\ &\quad \leqslant \sqrt{2(3+\sqrt{5})}||(I+A)^{-1/2}E_A([0,2\delta/\tau))u|| \\ &\qquad + \sqrt{\frac{3+\sqrt{5}}{2(1-m_f(\delta))}}||E_A([2\delta/\tau,\infty))u||\,\tau^{1/2} \end{aligned}$$

for $u \in \mathfrak{H}$ and $\tau>0$. Setting $C_A := \sqrt{2(3+\sqrt{5})}$ and $C_0 := \sqrt{\frac{3+\sqrt{5}}{2(1-m_f(\delta))}}$ we prove (3.1). $\square$

Lemma 4. *Let A and B be non-negative self-adjoint operators such that their form sum obeys* (1.2) *for some $\alpha \in (1/2, 1)$. Further, let f and g be Kato functions which satisfy* (1.3) *and* (1.4).

(i) *If $p, q \in [0, \alpha]$ and $p+q \geqslant 1$, then there is a constant $D_{p,q}>0$ such that*

$$||(I+H)^{-p}(H-S(\tau))(I+H)^{-q}|| \leqslant D_{p,q}\,\tau^{p+q-1} \tag{3.2}$$

for $\tau>0$.

(ii) *There is a constant $D_\alpha>0$ such that*

$$||S(\tau)(I+H)^{-\alpha}|| \leqslant D_\alpha\,\tau^{\alpha-1} \tag{3.3}$$

for $\tau>0$.

Proof. (i) First we note that if $p \in [0,\alpha]$, then condition (1.2) implies $\mathrm{dom}(H^p) \subseteq \mathrm{dom}(A^p) \cap \mathrm{dom}(B^p)$. Hence $(I+A)^p(I+H)^{-p}$ and $(I+B)^p(I+H)^{-p}$ are bounded operators. Since

$$\begin{aligned} I - F(\tau) = {} & I - f(\tau A/2)^2 + (I - g(\tau B)) \\ & + (I - f(\tau A/2))(I - g(\tau B))(I - f(\tau A/2)) \\ & - (I - f(\tau A/2))(I - g(\tau B)) - (I - g(\tau B))(I - f(\tau A/2)), \end{aligned} \tag{3.4}$$

we find

$$
\begin{aligned}
&(I+H)^{-p}(H-S(\tau))(I+H)^{-q}\\
&\quad = (I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q}\\
&\qquad + (I+H)^{-p}\left(B-\frac{I-g(\tau B)}{\tau}\right)(I+H)^{-q}\\
&\qquad - (I+H)^{-p}(I-f(\tau A/2))(I-g(\tau B))(I-f(\tau A/2))(I+H)^{-q}\tau^{-1}\\
&\qquad + (I+H)^{-p}(I-f(\tau A/2))(I-g(\tau B))(I+H)^{-q}\tau^{-1}\\
&\qquad + (I+H)^{-p}(I-g(\tau B))(I-f(\tau A/2))(I+H)^{-q}\tau^{-1},
\end{aligned}
$$

which gives the estimate

$$
\begin{aligned}
&\|(I+H)^{-p}(H-S(\tau))(I+H)^{-q}\|\\
&\quad \leqslant \left\|(I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q}\right\| \qquad (3.5)\\
&\quad + \left\|(I+H)^{-p}\left(B-\frac{I-g(\tau B)}{\tau}\right)(I+H)^{-q}\right\|\\
&\quad + \|(I-f(\tau A/2))(I+H)^{-p}\|\,\|(I-f(\tau A/2))(I+H)^{-q}\|\tau^{-1}\\
&\quad + \|(I-f(\tau A/2))(I+H)^{-p}\|\,\|(I-g(\tau B))(I+H)^{-q}\|\tau^{-1}\\
&\quad + \|(I-g(\tau B))(I+H)^{-p}\|\,\|(I-f(\tau A/2))(I+H)^{-q}\|\tau^{-1} \qquad (3.6)
\end{aligned}
$$

for $\tau > 0$. To estimate (3.5) we use

$$
\begin{aligned}
&\left\|(I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q}\right\|\\
&\quad \leqslant \|(I+A)^{p}(I+H)^{-p}\|\,\|(I+A)^{q}(I+H)^{-q}\|\\
&\qquad \times \left\|(I+A)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+A)^{-q}\right\|
\end{aligned}
$$

and the functional calculus which yield

$$\left\|(I+H)^{-p}\left(A-\frac{I-f(\tau A/2)^2}{\tau}\right)(I+H)^{-q}\right\|$$
$$\leqslant \|(I+A)^p(I+H)^{-p}\|\,\|(I+A)^q(I+H)^{-q}\|$$
$$\times\left\{|f|_{p+q}+\frac{1}{2}\gamma_f((p+q)/2)^2\right\}\tau^{p+q-1}$$

for $\tau>0$, where

$$\gamma_h(r) := \sup_{x>0}\frac{1-h(x)}{x^r}, \quad r\in(0,1],$$

and h is a Kato function. Similarly, one estimates (3.6) to get the inequality

$$\left\|(I+H)^{-p}\left(B-\frac{I-g(\tau B)}{\tau}\right)(I+H)^{-q}\right\|$$
$$\leqslant \|(I+B)^p(I+H)^{-p}\|\,\|(I+B)^q(I+H)^{-q}\|\,|g|_{p+q}\tau^{p+q-1}$$

for $\tau>0$. Since

$$\|(1-f(\tau A/2))(I+H)^{-r}\|\leqslant 2^{-r}\|(I+A)^r(I+H)^{-r}\|\,\gamma_f(r)\,\tau^r \tag{3.7}$$

and

$$\|(I-g(\tau B))(I+H)^{-r}\|\leqslant\|(I+B)^r(I+H)^{-r}\|\,\gamma_g(r)\,\tau^r \tag{3.8}$$

for $\tau>0$ and $r\in(0,\alpha]$, we finally obtain the estimate

$$\begin{aligned}
\|(I+H)^{-p}(H-S(\tau))(I+H)^{-q}\| &\leqslant \|(I+A)^p(I+H)^{-p}\| \\
&\times\|(I+A)^q(I+H)^{-q}\|\left\{|f|_{p+q}+\frac{1}{2}\gamma_f((p+q)/2)^2\right\}\tau^{p+q-1} \\
&+\|(I+B)^p(I+H)^{-p}\|\,\|(I+B)^q(I+H)^{-q}\|\,|g|_{p+q}\,\tau^{p+q-1} \\
&+\ 2^{-(p+q)}\gamma_f(p)\gamma_f(q)\|(I+A)^p(I+H)^{-p}\|\,\|(I+A)^q(I+H)^{-q}\|\,\tau^{p+q-1} \\
&+\ 2^{-p}\gamma_f(p)\gamma_g(q)\|(I+A)^p(I+H)^{-p}\|\,\|(I+B)^q(I+H)^{-q}\|\,\tau^{p+q-1} \\
&+\ 2^{-q}\gamma_f(q)\gamma_g(p)\|(I+A)^q(I+H)^{-q}\|\,\|(I+B)^p(I+H)^{-p}\|\,\tau^{p+q-1}
\end{aligned}$$

for $\tau > 0$. Setting

$$\begin{aligned}D_{p,q} := {}& ||(I+A)^p(I+H)^{-p}|| \\ & \times ||(I+A)^q(I+H)^{-q}||\left\{|f|_{p+q} + \frac{1}{2}\gamma_f((p+q)/2)^2\right\} \\ & + ||(I+B)^p(I+H)^{-p}||\,||(I+B)^q(I+H)^{-q}||\,|g|_{p+q} \\ & + 2^{-(p+q)}\gamma_f(p)\gamma_f(q)||(I+A)^p(I+H)^{-p}||\,||(I+A)^q(I+H)^{-q}|| \\ & + 2^{-p}\gamma_f(p)\gamma_g(q)||(I+A)^p(I+H)^{-p}||\,||(I+B)^q(I+H)^{-q}|| \\ & + 2^{-q}\gamma_f(q)\gamma_g(p)||(I+A)^q(I+H)^{-q}||\,||(I+B)^p(I+H)^{-p}||\end{aligned}$$

for $\tau > 0$ we prove the estimate (3.2).

(ii) Using decomposition (3.4) we find the estimate

$$\begin{aligned}& ||S(\tau)(I+H)^{-\alpha}|| \\ & \leqslant 4||(I-f(\tau A/2))(I+H)^{-\alpha}||\,\tau^{-1} + ||(I-g(\tau B))(I+H)^{-\alpha}||\,\tau^{-1}\end{aligned}$$

for $\tau > 0$. Taking into account (3.7) and (3.8) we obtain

$$\begin{aligned}||S(\tau)(I+H)^{-\alpha}|| \leqslant {}& 2^{2-\alpha}||(I+A)^\alpha(I+H)^{-\alpha}||\,\gamma_f(\alpha)\,\tau^{\alpha-1} \\ & + ||(I+B)^\alpha(I+H)^{-\alpha}||\,\gamma_g(\alpha)\,\tau^{\alpha-1}\end{aligned}$$

for $\tau > 0$. Setting

$$D_\alpha := 2^{2-\alpha}||(I+A)^\alpha(I+H)^{-\alpha}||\,\gamma_f(\alpha) + ||(I+B)^\alpha(I+H)^{-\alpha}||\,\gamma_g(\alpha)$$

we prove (3.3) for $\tau > 0$. $\square$

4. Error estimate

In order to prove the main theorem we need the following two lemmas.

Lemma 5. *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ condition* (1.2) *is satisfied. Further, let f and g be Kato functions which obey conditions* (1.3) *and* (1.4). *If in addition one has* $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ *and* $m_f(x) < 1$

for $x > 0$, *then there is a constant* $S_{\alpha-1/2} > 0$ *such that*

$$t\|(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \leqslant S_{\alpha-1/2}\left(\frac{\tau}{t}\right)^{\alpha-1/2} \tag{4.1}$$

for $t, \tau \in (0, 1]$ *with* $0 < \tau \leqslant t$.

Proof. By the functional calculus one has

$$\begin{aligned} &t\|(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \\ &\leqslant t^{1/2}\|(I + S(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \end{aligned}$$

for $t \in (0, 1]$ and $\tau > 0$. By Lemma 3 we find

$$\begin{aligned} &t\|(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \\ &\leqslant C_A \, \|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \, t^{1/2} \\ &\quad + C_0 \, \|(H - S(\tau))(I + tH)^{-1}\| \, \tau^{1/2} \, t^{1/2} \end{aligned} \tag{4.2}$$

for $t \in (0, 1]$ and $\tau > 0$. Since $\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2})$, we get

$$\begin{aligned} &\|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \\ &\leqslant \|(I + H)^{1/2}(I + A)^{-1/2}\| \, \|(I + H)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \end{aligned}$$

for $t \in (0, 1]$ and $\tau > 0$. Using again the functional calculus we obtain

$$\begin{aligned} &\|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \\ &\leqslant \|(I + H)^{1/2}(I + A)^{-1/2}\| \, \|(I + H)^{-1/2}(H - S(\tau))(I + H)^{-\alpha}\| \, t^{-\alpha} \end{aligned}$$

for $t \in (0, 1]$ and $\tau > 0$. By Lemma 4(i) there is a constant $D_{\frac{1}{2},\alpha} > 0$ such that

$$\begin{aligned} &\|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \\ &\leqslant D_{\frac{1}{2},\alpha} \, \|(I + H)^{1/2}(I + A)^{-1/2}\| \, \tau^{\alpha-1/2} \, t^{-\alpha}, \end{aligned}$$

which yields

$$\begin{aligned} &\|(I + A)^{-1/2}(H - S(\tau))(I + tH)^{-1}\| \, t^{1/2} \\ &\leqslant D_{\frac{1}{2},\alpha} \, \|(I + H)^{1/2}(I + A)^{-1/2}\| \left(\frac{\tau}{t}\right)^{\alpha-1/2} \end{aligned} \tag{4.3}$$

for $t \in (0, 1]$ and $\tau > 0$.

To estimate the second term of the right-hand side of (4.2), we use again the functional calculus to find that

$$||(H - S(\tau))(I + tH)^{-1}|| \leqslant \frac{1}{t} + ||S(\tau)(I + H)^{-\alpha}||\, t^{-\alpha}$$

for $t \in (0, 1]$ and $\tau > 0$. By virtue of Lemma 4(ii) there is a constant $D_\alpha > 0$ such that

$$||S(\tau)(I + tH)^{-1}|| \leqslant D_\alpha\, \tau^{\alpha-1}\, t^{-\alpha}$$

for $t \in (0, 1]$ and $\tau > 0$, which yields

$$||S(\tau)(I + tH)^{-1}||\, \tau^{1/2}\, t^{1/2} \leqslant D_\alpha \left(\frac{\tau}{t}\right)^{\alpha-1/2} \tag{4.4}$$

for $t \in (0, 1]$ and $\tau > 0$. Hence we obtain

$$||(H - S(\tau))(I + tH)^{-1}||\, \tau^{1/2}\, t^{1/2} \leqslant (1 + D_\alpha) \left(\frac{\tau}{t}\right)^{\alpha-1/2}$$

for $t, \tau \in (0, 1]$ and $0 < \tau \leqslant t$. Applying estimates (4.3) and (4.4) we find from (4.2) that

$$\begin{aligned} &t||(I + tS(\tau))^{-1/2}(H - S(\tau))(I + tH)^{-1}|| \\ &\leqslant \{C_A\, D_{\frac{1}{2},\alpha}||(I + H)^{1/2}(I + A)^{-1/2}|| + C_0(1 + D_\alpha)\}\left(\frac{\tau}{t}\right)^{\alpha-1/2} \end{aligned}$$

for $t, \tau \in (0, 1]$ with $0 < \tau \leqslant t$. Setting

$$S_{\alpha-1/2} \coloneqq C_A\, D_{\frac{1}{2},\alpha}\, ||(I + H)^{1/2}(I + A)^{-1/2}|| + C_0(1 + D_\alpha)$$

we get (4.1). $\square$

Lemma 6. *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ condition* (1.2) *is satisfied. Further, let f and g be Kato functions which obey conditions* (1.3) *and* (1.4). *Then there is a constant $G_{2\alpha-1} > 0$ such that*

$$t||(I + tH)^{-1}(H - S(\tau))(I + tH)^{-1}|| \leqslant G_{2\alpha-1}\left(\frac{\tau}{t}\right)^{2\alpha-1} \tag{4.5}$$

for $t \in (0, 1]$ and $\tau > 0$.

Proof. By the functional calculus we get

$$\begin{aligned} &t||(I + tH)^{-\alpha}(H - S(\tau))(I + tH)^{-\alpha}|| \\ &\leqslant ||(I + H)^{-\alpha}(H - S(\tau))(I + H)^{-\alpha}||\, t^{-(2\alpha-1)} \end{aligned}$$

for $t \in (0,1]$ and $\tau > 0$. Applying Lemma 4 we find a constant $G_{2\alpha-1} > 0$ such that

$$t\|(I+tH)^{-\alpha}(H-S(\tau))(I+tH)^{-\alpha}\| \leqslant G_{2\alpha-1}\left(\frac{\tau}{t}\right)^{2\alpha-1}$$

for $t \in (0,1]$ and $\tau > 0$, proving (4.5). $\square$

We are now going to prove the main theorem mentioned in the Introduction.

Proof of Theorem 1.1. By the resolvent identities

$$\begin{aligned}(I+tS(\tau))^{-1}-(I+tH)^{-1} &= t\,(I+tS(\tau))^{-1}(H-S(\tau))(I+tH)^{-1}\\ &= t\,(I+tH)^{-1}(H-S(\tau))(I+tS(\tau))^{-1}\end{aligned}$$

one gets

$$\begin{aligned}(I+tS(\tau))^{-1}-(I+tH)^{-1} &= t(I+tH)^{-1}(H-S(\tau))(I+tH)^{-1}\\ &\quad + t^2(I+tH)^{-1}(H-S(\tau))(I+tS(\tau))^{-1}\\ &\quad \times (H-S(\tau))(I+tH)^{-1}\end{aligned}$$

for $\tau, t > 0$. Hence we find the estimate

$$\begin{aligned}&\|(I+tS(\tau))^{-1}-(I+tH)^{-1}\|\\ &\quad\leqslant t\|(I+tH)^{-1}(H-S(\tau))(I+tH)^{-1}\|\\ &\qquad + t^2\|(I+tH)^{-1}(H-S(\tau))(I+tS(\tau))^{-1}(H-S(\tau))(I+tH)^{-1}\|\end{aligned}$$

for $\tau, t > 0$, which can be written as

$$\begin{aligned}&\|(I+tS(\tau))^{-1}-(I+tH)^{-1}\|\\ &\quad\leqslant t\|(I+tH)^{-1}(H-S(\tau))(I+tH)^{-1}\|\\ &\qquad + t^2\|(I+tS(\tau))^{-1/2}(H-S(\tau))(I+tH)^{-1}\|^2.\end{aligned}$$

Taking into account Lemmas 5 and 6 we get

$$\|(I+tS(\tau))^{-1}-(I+tH)^{-1}\| \leqslant G_{2\alpha-1}\left(\frac{\tau}{t}\right)^{2\alpha-1} + S^2_{\alpha-1/2}\left(\frac{\tau}{t}\right)^{2\alpha-1}$$

for $t, \tau \in (0,1]$ with $0 < \tau \leqslant t$. Setting $M_{2\alpha-1} := G_{2\alpha-1} + S^2_{\alpha-1/2}$ one gets a constant such that condition (2.4) holds for $\tau, t \in (0,1]$ with $0 < \tau \leqslant t$. By Theorem 2.1 there is a constant $C_{2\alpha-1} > 0$ such (2.5) is valid for $\varrho = 2\alpha - 1$ and $\tau, t \in (0,1]$ and $0 < \tau \leqslant t$. Setting $C_{1,2\alpha-1} := C_{2\alpha-1}$ and $\tau = t/n$, $n = 1, 2, \ldots$, we immediately verify (1.5) for $t \in [0,1]$.

To extend the result to $t \in [0, T]$, $0 < T < \infty$, we set $A_s := s\,A$ and $B_s := s\,B$ where $s > 0$. Obviously, one has $H_s := A_s \dot{+} B_s = s\,H$. If A and B are non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ condition (1.2) is satisfied, then, of course, one has $\mathrm{dom}(H_s^\alpha) \subseteq \mathrm{dom}(A_s^\alpha) \cap \mathrm{dom}(B_s^\alpha)$ for $s > 0$. Similarly, the condition $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ implies $\mathrm{dom}(A_s^{1/2}) \subseteq \mathrm{dom}(B_s^{1/2})$ for $s > 0$. Hence, there is a constant $C_{2\alpha-1}(s) > 0$ such that

$$||(f(tA_s/2n)g(tB_s/n)f(tA_s/2n))^n - e^{-tH_s}|| \leqslant C_{2\alpha-1}(s)\,\frac{1}{n^{2\alpha-1}}$$

for $t \in [0, 1]$ and $n = 1, 2, \ldots$, which yields

$$||(f(tA/2n)g(tB/n)f(tA/2n))^n - e^{-tH}|| \leqslant C_{2\alpha-1}(s)\,\frac{1}{n^{2\alpha-1}}$$

for $t \in [0, s]$ and $n = 1, 2, \ldots$. Choosing $s = T$ and setting $C_{T,2\alpha-1} := C_{2\alpha-1}(T)$ we get that for any finite interval $[0, T]$ there is a constant $C_{T,2\alpha-1} > 0$ such that (1.5) holds. $\square$

5. Related families

Let us show that estimate (6.1) holds not only for the family $F(\tau) = f(\tau A/2)g(\tau B)f(\tau A/2)$ but also for the families

$$F_1(\tau) := f(\tau A)^{1/2} g(\tau B) f(\tau A)^{1/2},$$

$$F_2(\tau) := g(\tau B)^{1/2} f(\tau A) g(\tau B)^{1/2},$$

$$F_3(\tau) := g(\tau B) f(\tau A),$$

$$F_4(\tau) := f(\tau A) g(\tau B),$$

$$F_5(\tau) := g(\tau B/2) f(\tau A) g(\tau B/2),$$

where $\tau \geqslant 0$. To this end we prove the following.

Lemma 7. *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ condition* (1.2) *is satisfied. Further, let f and g be Kato functions which obey* (1.3) *and* (1.4). *Then there is a constant $C_F > 0$ such that*

$$||(I - F(t/n))e^{-tH}|| \leqslant C_F\,\frac{e^t}{n^\alpha} \tag{5.1}$$

for $t \geqslant 0$ and $n = 1, 2, \ldots$.

Proof. We use the representation

$$(I - F(t/n))e^{-tH} = f(tA/2n)g(\tau B)(I - f(tA/2n))e^{-tH} + f(tA/2n)(I - g(tB/n))e^{-tH} + (I - f(tA/2n))e^{-tH},$$

which yields the estimate

$$\|(I - F(t/n))e^{-tH}\| \leqslant 2\|(I - f(tA/2n))e^{-tH}\| + \|(I - g(tB/n))e^{-tH}\|.$$

Since

$$(I - f(tA/2n))e^{-tH} = (I - f(tA/2n))(I + A)^{-\alpha}(I + A)^{\alpha}(I + H)^{-\alpha}(I + H)^{\alpha}e^{-(I+H)t}e^{t},$$

we find the estimate

$$\|(I - f(tA/2n))e^{-tH}\| \leqslant \|(I - f(tA/2n))(I + A)^{-\alpha}\| \, \|(I + A)^{\alpha}(I + H)^{-\alpha}\| \, \|(I + H)^{\alpha}e^{-(I+H)t}\| e^{t}.$$

Since

$$\|(I - f(tA/2n))(I + A)^{-\alpha}\| \leqslant \sup_{\lambda \geqslant 0} \frac{1 - f(t\lambda/2n)}{(1 + \lambda)^{\alpha}} \leqslant \sup_{\lambda > 0} \frac{1 - f(\lambda)}{\lambda^{\alpha}} \left(\frac{t}{2n}\right)^{\alpha} \leqslant \gamma_f(\alpha)\left(\frac{t}{2n}\right)^{\alpha},$$

we obtain the estimate

$$\|(I - f(tA/2n))e^{-tH}\| \leqslant 2^{-\alpha}\gamma_f(\alpha)b(\alpha)\|(I + A)^{\alpha}(I + H)^{-\alpha}\| \frac{e^{t}}{n^{\alpha}}$$

for $n = 1, 2, \dots$, where $b(\alpha) := \sup_{\lambda > 0} \lambda^{\alpha} e^{-\lambda}$. Similarly, we prove that

$$\|(I - g(tB/n))e^{-tH}\| \leqslant \gamma_g(\alpha)b(\alpha)\|(I + B)^{\alpha}(I + H)^{-\alpha}\| \frac{e^{t}}{n^{\alpha}}$$

for $n = 1, 2, \dots$. Setting

$$C_F := 2^{1-\alpha}\gamma_f(\alpha)b(\alpha)\|(I + A)^{\alpha}(I + H)^{-\alpha}\| + \gamma_g(\alpha)b(\alpha)\|(I + B)^{\alpha}(I + H)^{-\alpha}\|$$

one gets estimate (5.1). $\square$

Theorem 5.1. *Let A and B be non-negative self-adjoint operators such that for some $\alpha \in (1/2, 1)$ condition* (1.2) *is satisfied. Further, let f and g be Kato functions which satisfy conditions* (1.3) and (1.4). *If in addition one has* $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ *and $m_f(x) < 1$ for $x > 0$, then for any finite interval $[0, T]$ there are constants $C^{(j)}_{T,2\alpha-1} > 0$,*

$j = 1, 2, 3, 4, 5$, *such that*

$$||F_j(t/n)^n - e^{-tH}|| \leqslant C^{(j)}_{T,2\alpha-1} \frac{1}{n^{2\alpha-1}}, \quad j = 1, 2, 3, 4, 5 \tag{5.2}$$

for $t \in [0, T]$ *and* $n = 1, 2, \ldots$.

Proof. We set

$$f_0(x) := f(2x)^{1/2}, \quad x \geqslant 0.$$

The function $f_0(x)$ is also a Kato function which satisfies $|f_0|_{2\alpha} < \infty$ and $m_{f_0}(x) < 1$ for $x > 0$. One has

$$f_0(\tau A/2) = f(\tau A)^{1/2}, \quad \tau \geqslant 0. \tag{5.3}$$

We set

$$F_0(\tau) := f_0(\tau A/2) g(\tau B) f_0(\tau A/2), \quad \tau \geqslant 0.$$

By Theorem 1.1 there is a constant $C^{(0)}_{T,2\alpha-1} > 0$ such that

$$||F_0(t/n)^n - e^{-tH}|| \leqslant C^{(0)}_{T,2\alpha-1} \frac{1}{n^{2\alpha-1}}$$

for $t \in [0, T]$ and $n = 1, 2, \ldots$. By (5.3) one has $F_0(\tau) = F_1(\tau)$ for $\tau \geqslant 0$, which proves the assertion for $j = 1$. We note that

$$F_4(\tau)^n = f(\tau A)^{1/2} F_1(\tau)^{n-1} f(\tau A)^{1/2} g(\tau B), \quad \tau \geqslant 0, \quad n = 1, 2, \ldots .$$

Using the representation

$$\begin{aligned} F_4(\tau)^n - e^{-tH} = & f(\tau A)^{1/2} (F_1(\tau)^{n-1} (I - F_1(\tau)) f(\tau A)^{1/2} g(\tau B) \\ & + f(\tau A)^{1/2} (F_1(\tau)^n - e^{-tH}) f(\tau A)^{1/2} g(\tau B) \\ & + (f(\tau A)^{1/2} - I) e^{-tH} f(\tau A)^{1/2} f(\tau A)^{1/2} g(\tau B) \\ & + e^{-tH} (f(\tau A)^{1/2} - I) g(\tau B) + e^{-tH} (g(\tau B) - I), \end{aligned}$$

where $\tau = t/n$, $t \geqslant 0$ and $n = 1, 2 \ldots$, we find the estimate

$$\begin{aligned} ||F_4(\tau)^n - e^{-tH}|| \leqslant & ||F_1(\tau)^{n-1} (I - F_1(\tau))|| \\ & + ||F_1(\tau)^n - e^{-tH}|| + 2||(I - f(\tau A)^{1/2}) e^{-tH}|| + ||(I - g(\tau B)) e^{-tH}||. \end{aligned}$$

Since

$$||(I - f(\tau A)^{1/2})e^{-tH}|| \leqslant \gamma_f(\alpha)b(\alpha)||(I+A)^{\alpha}(I+H)^{-\alpha}||\frac{e^t}{n^{\alpha}} \tag{5.4}$$

and

$$||(I - g(\tau B)^{1/2})e^{-tH}|| \leqslant \gamma_g(\alpha)b(\alpha)||(I+B)^{\alpha}(I+H)^{-\alpha}||\frac{e^t}{n^{\alpha}} \tag{5.5}$$

as well as the estimate $||F_1(\tau)^{n-1}(I - F_1(\tau)|| \leqslant \frac{1}{n}$, $n = 1, 2, \ldots$, we obtain from the statement for $j = 1$ the existence of a constant $C^{(4)}_{T,2\alpha-1} > 0$ such that (5.2) holds for $j = 4$, $t \in [0, T]$ and $n = 1, 2, \ldots$. Next, using

$$F_3(\tau)^n = g(\tau B)F_4(\tau)^{n-1}f(\tau A)$$

and

$$F_2(\tau)^n = g(\tau B)^{1/2}F_4(\tau)^{n-1}f(\tau A)g(\tau B)^{1/2}$$

$\tau \geqslant 0$, $n = 1, 2, \ldots$, as well as estimates (5.4) and (5.5) one verifies (5.2) for $j = 2, 3$ in the same way as above. To prove the statement for $j = 5$ we introduce the function

$$g_0(x) := g(x/2)^2, \quad x \geqslant 0.$$

Then one gets $F_5(\tau) = g_0(\tau B)^{1/2}f(\tau A)g_0(\tau B)^{1/2}$ for $\tau \geqslant 0$. The function g_0 is again a Kato function which satisfies (1.4). Hence, applying here the result for $F_2(\tau)$ we prove the case $j = 5$. $\square$

6. Example

Let $\mathfrak{H} := L_2(\Omega)$ where Ω is a bounded domain in $\mathbb{R}^l$, $l = 1, 2, \ldots$, with boundary $\partial\Omega$ of C^∞-class. By A we denote the negative half Laplacian with Dirichlet boundary conditions on $L_2(\Omega)$, i.e $A = -\frac{1}{2}\Delta_D$. The domain is given by

$$\mathrm{dom}(A) := H^2_2(\Omega) \cap \mathring{H}^1_2(\Omega),$$

where $\mathring{H}^1_2(\Omega)$ is the closure of $C^\infty_0(\Omega)$ in the Lebesgue space $H^1_2(\Omega)$, cf. Definitions 4.2.1/1 and 4.2.1/2 of [18]. Using the space $H^2_{2,B_D}(\Omega)$,

$$H^2_{2,B_D}(\Omega) := \{u \in H^2_2(\Omega) \colon \; B_D u|_{\partial\Omega} = 0\},$$

cf. Definition 4.3.3/2 of [18], where B_D is given by

$$B_D u := u|_{\partial\Omega}$$

for $u \in H_2^2(\Omega)$, we obtain

$$\mathrm{dom}(A) := H^2_{2,B_D}(\Omega).$$

Further, let B be the negative half Laplacian with Neumann boundary conditions, i.e $B := -\frac{1}{2}\Delta_N$. One has

$$\mathrm{dom}(B) := H^2_{2,B_N}(\Omega),$$

where

$$H^2_{2,B_N}(\Omega) := \{u \in H^2_2(\Omega) \colon\ B_N u|_{\partial\Omega} = 0\},$$

cf. Definition 4.3.3/2 of [18]. The boundary operator B_N is given by

$$(B_N u)(x) = \frac{\partial}{\partial v(x)} u(x), \quad x \in \partial\Omega,$$

for $u \in H_2^2(\Omega)$ where $v(x)$ is the outer unit normal to the boundary $\partial\Omega$ at the point $x \in \partial\Omega$. Since $\mathrm{dom}(A^{1/2}) = \mathring{H}^1_2(\Omega)$ and $\mathrm{dom}(B^{1/2}) = H^1_2(\Omega)$ one gets

$$\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2}).$$

Hence

$$\mathrm{dom}(H^{1/2}) = \mathrm{dom}(A^{1/2}) \cap \mathrm{dom}(B^{1/2}) = \mathring{H}^1_2(\Omega).$$

and $H := A \dot{+} B = 2A = -\Delta_D$. Therefore $\mathrm{dom}(H^\alpha) = \mathrm{dom}(A^\alpha)$ for arbitrary $\alpha \in [0, 1]$.

Now we are going to calculate the domains $\mathrm{dom}(A^\alpha)$ and $\mathrm{dom}(B^\alpha)$ for $\alpha \in (1/2, 1)$. By Theorem 1 and Theorem 2 of [4] and Theorem 8.1 of [5] (see also Theorem 4.3.3 of [18]) we find

$$\mathrm{dom}(A^\alpha) = H^{2\alpha}_{2,B_D}(\Omega), \quad \alpha \in (1/2, 1),$$

and

$$\mathrm{dom}(B^\alpha) = \begin{cases} H_2^{2\alpha}(\Omega), & \alpha \in (1/2, 3/4), \\ H^{2\alpha}_{2,B_N}(\Omega), & \alpha \in (3/4, 1). \end{cases}$$

Since $H^{2\alpha}_{2,B_D}(\Omega) \subseteq H^{2\alpha}_2(\Omega)$ one gets

$$\mathrm{dom}(H^\alpha) = \mathrm{dom}(A^\alpha) \subseteq \mathrm{dom}(B^\alpha)$$

for $\alpha \in (1/2, 3/4)$. Applying now Theorem 5.1 we find that

$$||(e^{-t(-\Delta_D)/2n}e^{-t(-\Delta_N)/2n})^n - e^{-t(-\Delta_D)}|| = O(n^{-\kappa})$$

for any $\kappa := 2\alpha - 1 < \kappa_0 := \frac{1}{2}\ (\alpha < \frac{3}{4})$ uniformly in $t \in [0, T]$ as $n \to \infty$.

If $\alpha = 3/4$, then it does not hold that $\mathrm{dom}(A^{3/4}) \subseteq \mathrm{dom}(B^{3/4})$. Hence $\mathrm{dom}(A^{3/4}) \cap \mathrm{dom}(B^{3/4})$ is a proper subset of $\mathrm{dom}(H^{3/4})$ which does not allow one to apply Theorem 5.1.

If $\alpha \in (3/4, 1)$, then

$$\begin{aligned}\mathrm{dom}(A^{\alpha}) \cap \mathrm{dom}(B^{\alpha}) &= H^{2\alpha}_{2,\{B_D,B_N\}}(\Omega) \\ &:= \{u \in H^{2\alpha}_2(\Omega) : B_D u|_{\partial\Omega} = 0, B_N u|_{\partial\Omega} = 0\} \subseteq H^{2\alpha}_{2,B_D}(\Omega).\end{aligned}$$

This yields that $\mathrm{dom}(A^{\alpha}) \cap \mathrm{dom}(B^{\alpha})$ is a proper subset of $\mathrm{dom}(H^{\alpha})$ which does not allow one to apply Theorem 5.1, either.

If $\alpha = 1$, then one gets that $\mathrm{dom}(A) \cap \mathrm{dom}(B)$ is a proper subset of $\mathrm{dom}(H)$ too which yields $H \neq A + B$. Therefore the results of [11,12] are not applicable.

Notice that in contrast to [14] and to examples given there, here we have given an example when the operator B^{α} is not small with respect to A^{α} for $\alpha \in (1/2, 3/4)$.

7. Remarks

Let us make the following remarks:

(i) By an example given in [17] the error bound estimate $O(n^{-(2\alpha-1)})$ in Theorems 1.1 and 5.1 cannot be improved, i.e. it is the *ultimate optimal* one.

(ii) This optimal error bound was already found in [14] see Theorems 5.3 and 5.5. In comparison with [14] the conditions on the operators A and B are relaxed here. There it was assumed that B^{α} is small with respect to A^{α}, i.e. $\mathrm{dom}(A^{\alpha}) \subseteq \mathrm{dom}(B^{\alpha})$ and

$$||B^{\alpha}u|| \leqslant a||A^{\alpha}u|| + b||u||, \quad u \in \mathrm{dom}(A^{\alpha}), \tag{7.1}$$

for some $\alpha \in (1/2, 1)$ and $a \in (0, 1)$, $b > 0$. This condition is reduced in the present paper to the mild subordination condition $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$, which (7.1) obviously implies. The yet open problem is to eliminate completely this subordination condition.

(iii) The conditions on the Kato functions f and g are essentially relaxed compared with [14]. Indeed, in [14] the Kato functions f and g have to satisfy at zero a smoothness condition of the type $|f|_2, |g|_2 < \infty$ which is replaced here by $|f|_{2\alpha}, |g|_{2\alpha} < \infty$, $\alpha \in (1/2, 1)$. A behavior at infinity like $f(x) \sim x^{-2\alpha}$ is also demanded there.

(iv) Theorem 1.1 shows that only relations between certain domains related to A, B and H are decisive for the *convergence rate* of the Trotter–Kato product formula.
(v) Theorem 1.1 holds for $\alpha \in (1/2, 1)$. The method of the proof does not allow one to include the case $\alpha = 1$. However, this case was considered in [11,12]. It is remarkable that one does not need any subordination condition there.
(vi) For $\alpha = 1/2$ we cannot expect operator-norm convergence in general, see [17]. However, if there is a subordination such that the operator B is relatively compact with respect to A, then operator-norm convergence holds, see [15].

The first version of this result was announced in [8] with a sketch of a proof which relies on an operator-norm estimate proved by Birman and Solomyak in [1]. In the present paper we have improved this previous result, by removing some restrictive condition on the Kato functions f and g imposed there as well as by giving a different, simpler proof which does not make use of operator-norm inequalities à la Birman–Solomyak.

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